Fluoropropanate-sodium

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 5.83 °C

Global applicability domain: Inside

Local applicability domain index: 4.53e-01

Confidence level: 6.21e-01

Nearest Neighbors from the Training Set

Image not found
Acetic acid, difluoro-
Measured: -1.00
Predicted: 19.4

Image not found
Acetic acid, trifluoro-
Measured: -15.2
Predicted: -15.5

Image not found
1-Propanol, 2,2,3,3-tetrafluoro-
Measured: -15.0
Predicted: -15.0

Image not found
2-(Trifluoromethyl)acrylic acid
Measured: 51.5
Predicted: 57.7

Image not found
Acetic acid, chlorodifluoro-
Measured: 25.0
Predicted: 33.2